REPORT DOCUMENTATION PAGE	Form Approved OMB No. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
22/Sept/06	Final Technical	01/Sept/01-30/Sept/05

4. TITLE AND SUBTITLE
Development of an Accelerated Methodology for the Evaluations of Critical Mechanical Properties of Polyphase Alloys by Simulation and Experiment

5a. CONTRACT NUMBER F49620-02-1-0047
5b. GRANT NUMBER
5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
Paul Dawson
Matthew Miller
Tong-Seok Han
Joel Bernier

5d. PROJECT NUMBER
5e. TASK NUMBER
5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Cornell University

8. PERFORMING ORGANIZATION REPORT NUMBER
None

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Air Force Office of Scientific Research

10. SPONSOR/MONITOR'S ACRONYM(S)
AFOSR

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release, distribution unlimited

AFRL-SR-AR-TR-06-0389

13. SUPPLEMENTARY NOTES
None

14. ABSTRACT

A system for more rapidly determining the strength and stiffness of polyphase alloys was developed that is based on a digital representation of the material structure. Working in concert with the representation are a number of digital tools and probes that are analogues of testing equipment and instrumentation of traditional laboratory methods. These are combined with nontraditional mechanical testing methods to complete the system. An example of an iron-copper (Fe-Cu) system is used to illustrate the methodology.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
u	u	u	uu		Paul Dawson
					19b. TELEPHONE NUMBER (Include area code) 607-255-3466

DEVELOPMENT OF AN ACCELERATED METHODOLOGY FOR THE EVALUATIONS OF CRITICAL MECHANICAL PROPERTIES OF POLYPHASE ALLOYS BY SIMULATION AND EXPERIMENT

F49620-02-1-0047

Paul Dawson
Sibley School of Mechanical and Aerospace Engineering
Cornell Univeristy

Matthew Miller
Sibley School of Mechanical and Aerospace Engineering
Cornell Univeristy

Tong-Seok Han
Sibley School of Mechanical and Aerospace Engineering
Cornell Univeristy

Joel Bernier
Sibley School of Mechanical and Aerospace Engineering
Cornell Univeristy

Abstract
A system for more rapidly determining the strength and stiffness of polyphase alloys was developed that is based on a digital representation of the material structure. Working in concert with the representation are a number of digital tools and probes that are analogues of testing equipment and instrumentation of traditional laboratory methods. These are combined with nontraditional mechanical testing methods to complete the system. An example of an iron-copper (Fe-Cu) system is used to illustrate the methodology.

1 Introduction

The need to expedite material development is broadly recognized and currently being addressed via a number of directed research programs. Two presumptions are made across much of this work. First, it is the mechanical properties that must be known to designers. To ascertain the properties more rapidly, a more quantitative understanding of the dependence of properties on features of the structure is essential. Second, by augmenting the traditional laboratory tools with a combination of computer modeling and non-traditional tests, the overall development time could be shortened.

The methodology developed under this grant facilitates more rapid material development. We are focused on the more rapid determination of the strength and stiffness of polyphase alloys using a combination of simulation and experiment based with the aid of a quantitative association between critical features of the structure and the mechanical response.

The model material we use to demonstrate the methodology is a mechanically-alloyed and HIP-sintered system composed of equal volume fractions of iron and copper. This material system forms a two-phase alloy in which each phase is comprised purely of a single constituent. SEM-generated images of the Fe/Cu - 50/50 alloy is shown if Figure 1 along with the electron backscattered data depicting the grain structure for each phase. Some feature attributes relevant to the strength and stiffness of a polyphase alloy, as well as the probes used to obtain them are listed in Table 1. We also investigated two-phase system consisting of aluminum and beryllium. We anticipate that the data for this system, also cast in the Digital Material framework, will be available later.

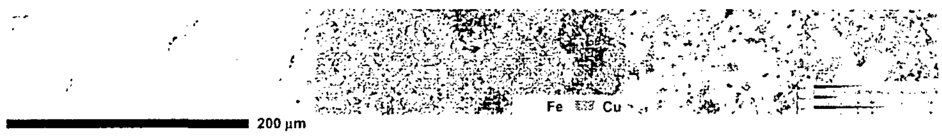


Figure 1: (Left) Secondary electron image of a region in the 50/50 Fe/Cu alloy specimen. (Middle) EBSD generated phase map of the same region showing areas of iron and coper. (Right) EBSD crystal lattice orientation map where individual grains within each phase are denoted by regions of like color.

Feature	Attribute	Physical Probe	Virtual Probe
Phase	volume fraction	neutron and x-ray diffraction	sectioning probe
	crystal structure	EBSD, neutron and x-ray diffraction	N/A
	contiguity	EBSD, (serial) sectioning	contiguity probe
Grain	morphology	EBSD, (serial) sectioning	sectioning probe
	ODF	EBSD, neutron and x-ray diffraction	discrete orientations
	MODF	EBSD, neutron and x-ray diffraction	discrete orientations
	lattice strains	neutron and x-ray diffraction	diffraction probe
Derived Properties		**Physical Probe**	**Virtual Probe**
Strength		Mechanical tests	Loading tools (flow surface)
Stiffness		Mechanical tests	Loading tools (directional modulus)

Table 1: Features and attributes for the Digital Material representation of a two-phase alloy

2 The Digital Material

As the joint focus of the testing and modeling efforts is on the material, it is useful to employ a quantitative description of the material itself as the unifying entity of the Digital Material system. For this purpose, we introduced the Digital Material, a feature-based representation of the material, and built the system around its existence. The complete system includes numerical capabilities to create a virtual specimen, mechanically load it, and measure its response. These capabilities are referred to as specimen instantiation, tools, and probes, and are analogous to samples of the material, testing apparati, and instrumentation, respectively.

2.1 Features and Attributes

For the strength and stiffness, we include the phases, the grains, dislocation structure, grain boundaries and particles. One could continue to add features of smaller characteristic dimensions, like precipitates, but for now we truncated the representation here at the level of constituent particles. The decision of what level of detail is to be included in the representation is important.

Every attribute distribution must be described mathematically. To do this, one needs to specify a parametrization, that is a choice of variables, and a representation, that is a choice of functions. The choices are not unique and often several combinations work equally well. To standardize the representations of attributes within the Digital Material, we fixed on the use of piecewise polynomial functions for all of the distributions regardless of the choice of parametrization. This choice provides a number of advantages, but particularly influential are the uniformity it brings across the full array of features and attributes and the efficiency it affords in computations associated with sampling and averaging. The particular type of polynomial functions we use are those referred to in finite element methods as low-order, isoparametric, Lagrange elements.

2.2 Database structure

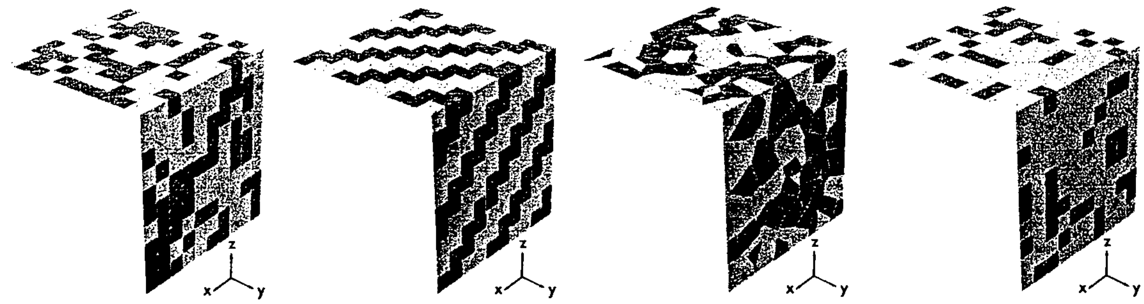
The Digital Material is a central repository for what is known about the structural state of a material. Individuals working on or with a material can communicate their knowledge about that material through the Digital Material. For this reason it is important to store this information in a manner that assures accurate, reliable records, yet facilitates easy access for a variety of uses. Modern database systems provide the necessary functionality for this purpose.

The database was designed to handle an arbitrary number of states for a given material. The Digital Material distinguishes between the material itself and the properties it exhibits. The material is defined by the features and attributes it is assigned. The properties correspond to the response samples of the material display under various types of loading (stimuli). Thus, properties are not part of the material *per se*, but rather reside in an appendix that is attached to the material. The representation of properties is discussed in a later subsection.

2.3 Virtual Experimental Environment

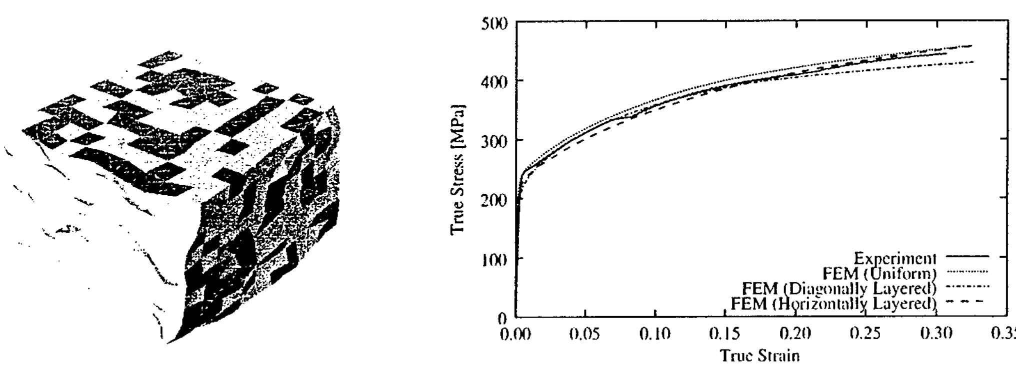
The complete Digital Material system mimics a laboratory-based system for the evaluation of mechanical properties. Just as in the physical case, the material is distinct from the tools that operate on it or the instrumentation that monitors its response. In addition to the material representation (the Digital Material), the system includes a number of other components that are numerical analogues of traditional testing capabilities. These fall into one of several broad categories listed below.

Digital Specimen Cutters provide the means to instantiate a virtual specimen using state data sampled from attribute distributions in the Digital Material and are analogous to machining a specimen from stock. The specimen instantiation method generates crystals with regular dodecahedral geometries and discretizes each crystal with 48 higher-order tetrahedral finite elements. Figure 2 depicts several instantiated 50/50 Fe/Cu specimens. The main objective for the instantiation process is creation of a virtual specimen or specimens that have distributions of the relevant geometric attributes that are statistically consistent with those measured in the actual microstructure.



(a) (b) (c) (d)

Figure 2: Four different instantiations, (a) Fe/Cu-50/50 volume fraction, random phase distribution, rhombic dodecahedral tessellation, (b) Fe/Cu-50/50 volume fraction, diagonally layered phase distribution, rhombic dodecahedral tessellation, (c) Fe/Cu-50/50 volume fraction, random phase distribution, random Voronoi tessellation, (d) Fe/Cu-67/33 volume fraction, random phase distribution, rhombic dodecahedral tessellation (Cu-phase: blue, Fe-phase: red)



(a) (b)

Figure 3: Deformed mesh (a) and mechanical response (b) Cu-phase following compression of the specimen with uniform contiguity of equal volume fraction to a true strain of 34%

Digital Tools provide the means to operate on a virtual specimen drawn from the material representation. One tool is a finite element code that simulates the deformation of a virtual specimen and is analogous to a load frame. Figure 3 shows a finite element-based specimen compressed to a true strain of 34% under uniaxial stress to illustrate the possible modification in state induced by a processing operation. The heterogeneity of the deformation caused by differences in phase properties is evident. Figure 3 also shows the computed stress-strain response over the course of the loading.

Digital Probes provide the means to characterize the state of a virtual specimen and to interrogate (measure) its behavior under loading. Contiguity is a measure of phase percolation, which is an important factor for both strength and stiffness. Figure 4 illustrates how the continuity is computed. Starting with a virtual specimen, a bundle of rays are passed through the specimen. Along each ray, statistics are collected related

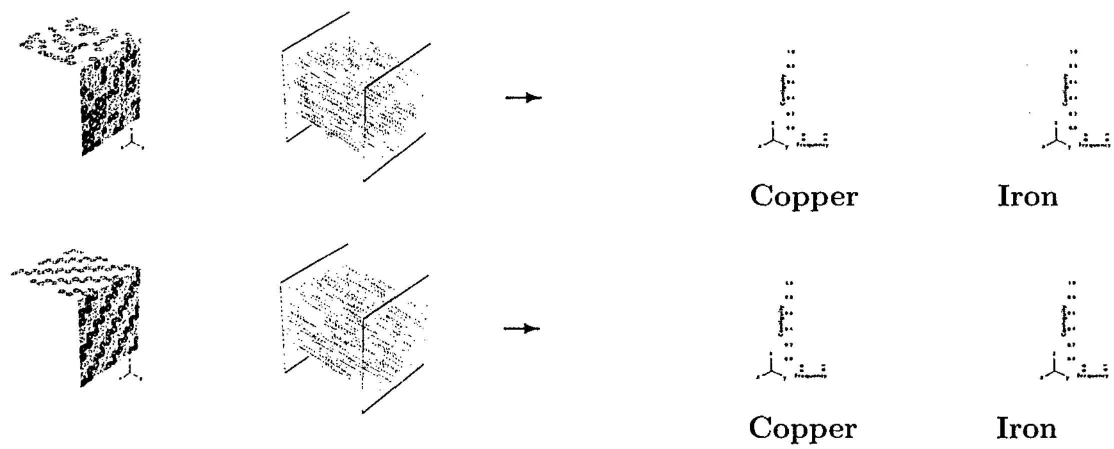


Figure 4: Illustration of the digital probe for quantifying the contiguity of two-phase specimens comprised of dodecahedral grains of differing topology. The color of a point on the sphere represents the contiguity associated with a probe direction (direction of the ray bundle) corresponding to the direction normal to the sphere at that point. The color bar provides the scale for the color map and the additional information in the form of a histogram of the frequency distribution of the corresponding values of the contiguity

to whether or not a different phase is encountered when the ray leaves one crystal and enters another. The contiguity value varies between zero and unity. A value of zero indicates that on passing from one crystal to another, the ray always enters a different phase. A value of unity indicates that the ray always enters a crystal of the same phase when it passes over a grain boundary. The process is repeated for rays in all directions, giving a distribution of contiguity defined over the surface of a sphere. The initial contiguity for each phase in this specimen was the average value of 0.5 and uniformly distributed. Figure 5 illustrates the continuity following the compressive deformation shown in Figure 3.

A virtual diffraction probe has been constructed that mimics a physical diffractometer by identifying those crystals that satisfy a specific Bragg condition. This allows for the comparison of simulated mechanical response to that measured during *in situ* tests. The grains selected by the virtual diffractometer can be queried for lattice strains, which can be compared to experimental results, as depicted in Figure 6.

2.4 The Digital Material Properties Appendix

The basic objective in building and applying the Digital Material system is to accelerate the determination of the strength and stiffness of polyphase alloys. For any combination of material and state, the strength and stiffness must be determined and recorded in a way that is useful to designers. To facilitate this, an appendix to the Digital Material has been created that holds this vital information. As with the attributes of the Digital Material, we employ a numerical representation of the distributions of stiffness and strength, with values computed by loading the virtual specimens with appropriate combinations of the Digital Tools. Again,

(a) (b)

Figure 5: Contiguities ((a) Cu-phase, (b) Fe-phase) following compression of the specimen with uniform contiguity of equal volume fraction to a true strain of 34%

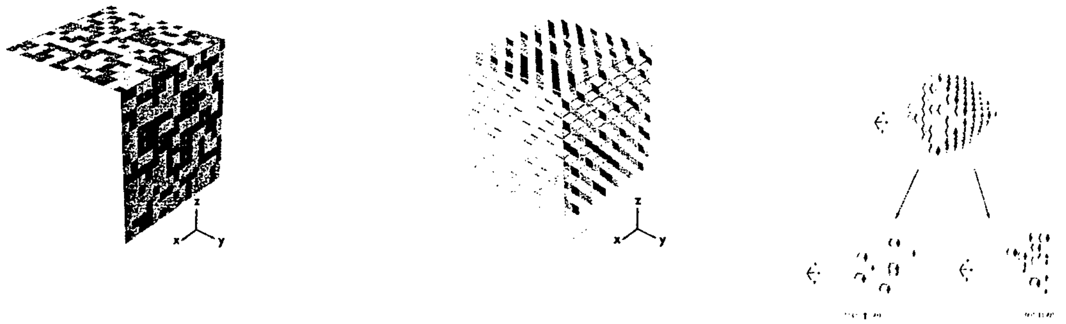


Figure 6: Illustration of identifying crystals that satisfy a particular Bragg condition using the digital diffraction probe. Shown are the complete specimen (left), the inner set of complete dodecahedral grains (center), and an arbitrary diffraction volume (right). Two Bragg conditions are shown: grains whose 111 normals align with the the 001 sample direction and grains whose 100 normals align with the the 001 sample direction. Blue grains are copper phase; red grains are iron phase. The diffraction peaks would be distinct for the two phases provided that the lattice parameters (plane spacings) are different.

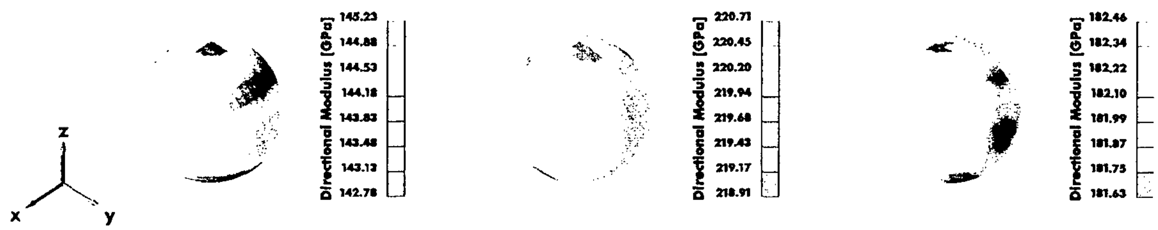


Figure 7: Directional stiffness distributions for each phase of an iron-copper alloy.

visualization is important. Here we show the result of computing the directional flow stress for the deformed Fe-Cu material using tools that deliver the upper bound. The color scale indicates the magnitude of the flow stress:

$$\bar{\sigma}' = \|\boldsymbol{\sigma}'\| = \mathrm{f}(d_1, d_2, d_3, d_4, d_5) \tag{1}$$

as a function of the deformation rate, recording as a five-dimensional vector:

$$(d_1, d_2, d_3, d_4, d_5) = \Big((D'_{22} - D'_{11}), \sqrt{3}D'_{33}, 2D'_{23}, 2D'_{31}, 2D'_{12}\Big) / \sqrt{2}. \tag{2}$$

3 Physical experiments

The primary role of the experimental data within the Digital Material system is the establishment of reference states. These are direct points of contact between measured and calculated attribute values for the same nominal material state. As such, the reference state fulfills a critical dual purpose: it provides the bases for model initialization as well as validation. For generality the attribute data must be comprised of physically measurable quantities. In addition, the experiments must provide enough information to extract statistical attribute distributions for the relevant features. This often requires the modification and combination of traditional experimental methods.

One attribute of the grains (see Table 1) that we employed extensively in this work is lattice strain. We see this as a direct link to the micromechanical state - making it invaluable for model validation. Significant work has focused on the development of lattice strain measurement techniques using both neutrons and synchrotron x-rays. Each technique has its advantages. Lattice strains measured using Time of Flight (TOF) neutrons at the SMARTS instrument at Los Alamos National Labs are highly resolved and extremely reliable. The x-ray measurements made at CHESS at Cornell allow for the simultaneous collection of lattice strains for many families of planes along many scattering vectors. The experimental setup for performing in situ diffraction experiments is shown in Figure 9(a). By rotating the loading stage, strain data can be collected over a range of scattering vectors. These data populate a strain pole figure, such as that shown in Figure 9(b), for each phase at each load.

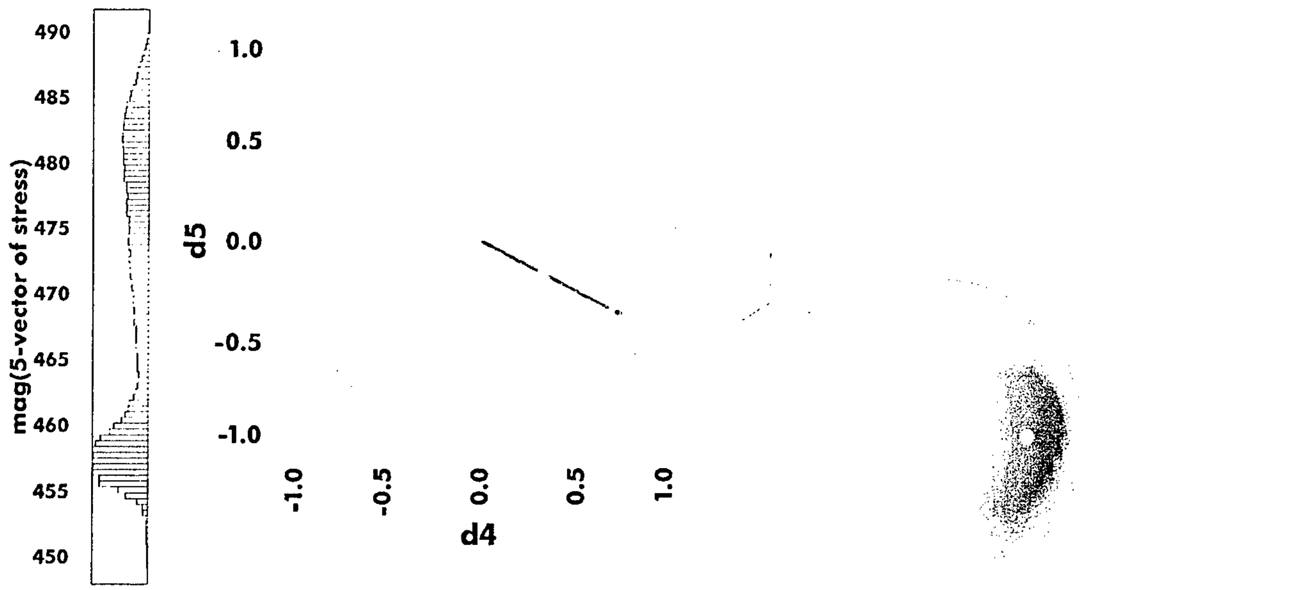


Figure 8: Directional strength distributions for each phase of an iron-copper alloy.

A procedure was developed to invert the data from multiple pole figures to produce a Lattice Strain Distribution Function. An example of these distributions is shown for the copper phase of the iron-copper system in Figure 10 for increasing levels of load. This representation gives the full lattice strain tensor at every point in orientation space. Figure 11 shows experimental and simulated lattice strain results. The finite element results compare well to the measured values. The predicted lattice strain tensor is shown in Figure 11 for crystal orientations that contribute to the average strain shown in the comparison. Here, the strain jacks depict the full strain tenor with the colors indicating magnitudes of principal values and the orientation indicating principal directions. The strain jacks are not all oriented the same way, indicating that the lattice strains differ from crystal to crystal, depending in part on the orientation of the crystal's lattice. The departure from a uniaxial deformation state in the copper is obvious in both figures.

4 Visualizing the Digital Material and its Property Appendix

It is envisioned that the material designer will iterate using the Digital Material since material attributes and properties from additional material states that may be more difficult and costly to realize physically can be analyzed much more efficiently in the virtual realm. Graphical User Interfaces (GUIs) were created as a means for the designer to visualize the attributes associated with the Digital Material. Figure 12 depicts a screenshot of the GUI used to examine the ODF of the copper phase in the 50/50 alloy. A GUI also was developed for viewing information in the properties appendix. Figure 13 depicts a screenshot of the GUI used to understand flow stress variations as a function of the material anisotropy and the applied strain rate.

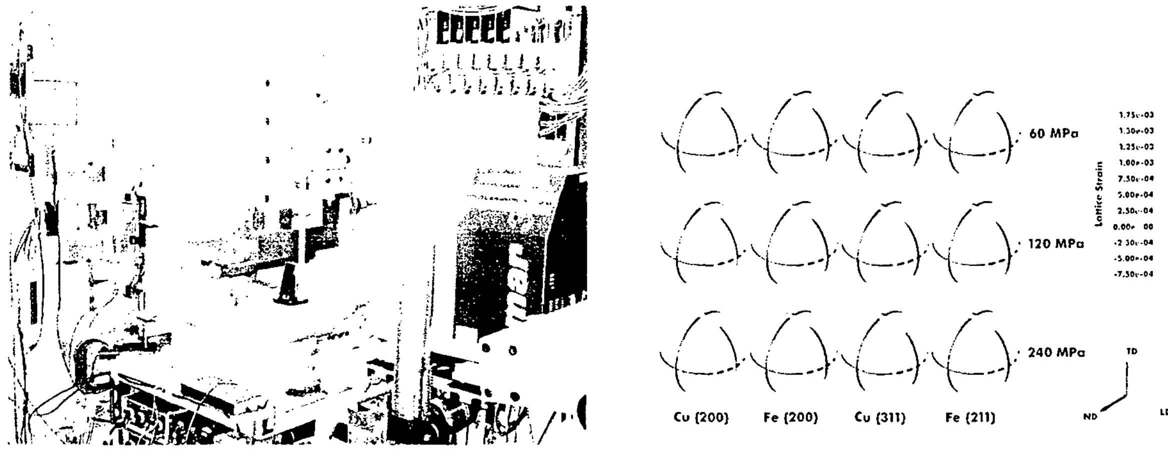


Figure 9: Left: experimental diffractometer for measuring lattice strains under load. Right: lattice strain pole figures produced from the CHESS data showing the progression of straining during the in-situ mechanical loading experiment.

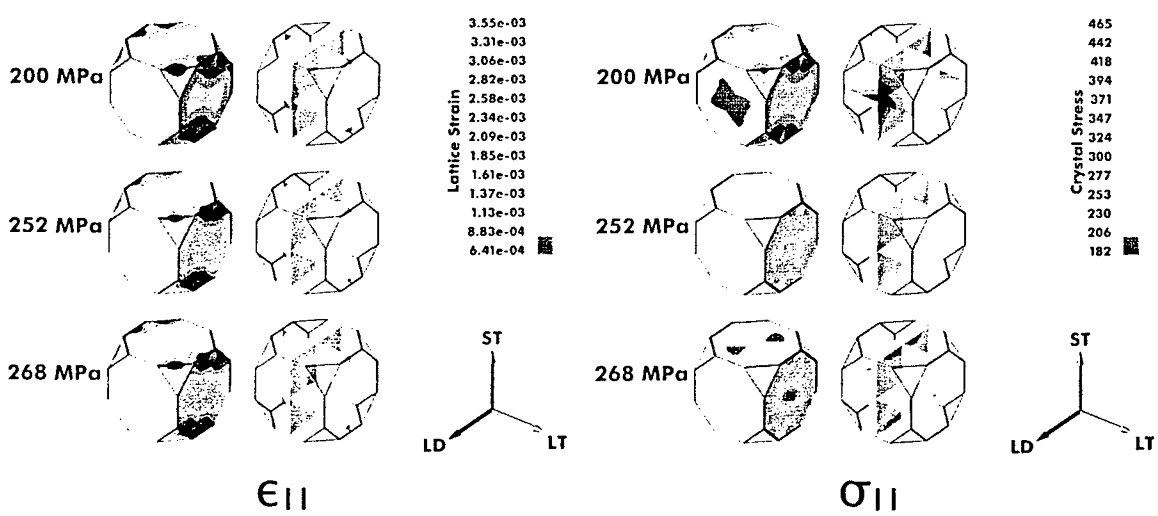
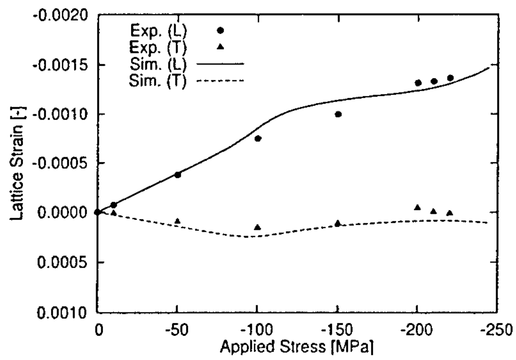
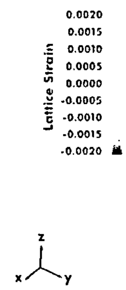


Figure 10: Left: lattice strain distribution functions for one normal strain component in the copper phase at several load levels. Right: normal stress component computed using the full strain tensor shown on the left.



(a)



(b)

Figure 11: (a): Simulated and measured lattice strains for the 200 families of copper crystals in the Fe/Cu 50/50 alloys during compression (L: Loading direction, T: Transverse direction). (b): Simulated lattice strain tensor visualization using "jacks" at an applied uniaxial stress of 248 MPa. The orientation of the principal strain axes comprise the form of the jack with the color related to the magnitude. The jacks on the fiber along the z-axis represent lattice strains of {200} crystals along the loading direction, and jacks on the fiber along the x-axis represent lattice strains of {200} crystals transverse to the loading direction.

5 Documentation of Results – Publications

A number of archival publications were completed that document various aspects of the research. These include articles on the Digital Material framework, representation of attributes like contiguity, the Digital Tool (finite element analyses for the mechanical response under loading), and physical experiments (new in situ diffraction methods). Articles in print at the conclusion of the project listed below. A couple other articles were still in progress at the time the final report was compiled.

1. P. R. Dawson, M. P. Miller, T.-S. Han, and J. Bernier. An accelerated methodology for the evaluation of critical properties in polyphase alloys, **Metallurgical and Materials Transactions**, 36A:1627–1641, 2005.

2. T.-S. Han and P. R. Dawson, Representation of anisotropic phase morphology, **Modeling and Simulation in Materials Science and Engineering**, 13(2):203–223, 2005.

3. T.-S. Han and P. R. Dawson. Lattice strain partitioning in a two-phase alloy and it redistribution upon yielding, **Materials Science and Engineering A**, 405:18–33, 2005.

4. M. P. Miller, J. V. Bernier, and J.-S. Park. Experimental measurement of lattice strain pole figures using synchrotron x-rays. **Rev. Sci. Instrum.** 76:113903-113913, 2005.

5. J. V. Bernier and M. P. Miller. A Direct Method for Determining the Orientation-Dependent Distribution of Lattice Strains for Strain Pole Figures. **Journal of Applied Crystallography** 39:358-368, 2006.

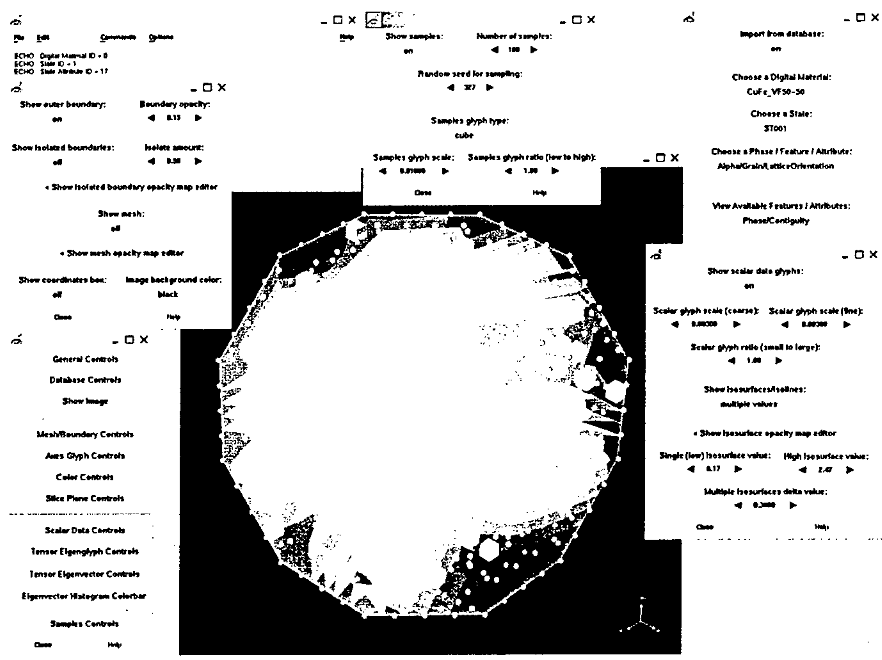


Figure 12: GUI used to depict the Crystal ODF within the Digital Material. (Note: In the image window at the center, the ODF for cubic fundamental region is visualized using small sphere glyphs at nodal points and iso-surface contours. The cubes correspond to randomly selected orientations used to instantiate a virtual specimen.)

6. J. V. Bernier, M. P. Miller, and D. E. Boyce. A Novel Optimization-Based Pole Figure Inversion Method: Comparison with WIMV and Maximum Entropy Methods. **Journal of Applied Crystallography** 39:697-713. 2006.

7. T.-S. Han and P. R. Dawson. A two-scale deformation model for polcrystalline solids using a strongly-coupled finite element methodology, **Computer Methods is Applied Mechanics and Engineering**, in press

6 Personnel Supported

The individual who received support under this grant were:

Paul R. Dawson	Professor, Cornell University
Matthew P. Miller	Associate Professor, Cornell University
Tong-Seok Han	Postdoc, Cornell University
Joel Bernier	Graduate Student, Cornell University

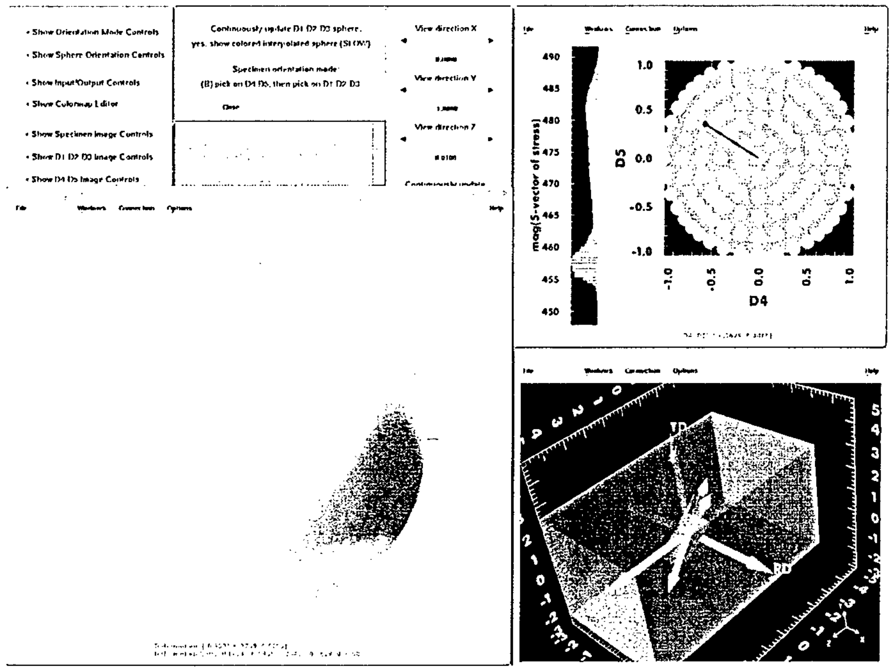


Figure 13: GUI used to access flow strength in five-dimensional deformation rate space. The fourth (d_4) and fifth (d_5) components of the five-dimensional vector form of deformation rate are selected interactively from the image panel on the upper right corner. Then the magnitudes of the flow strengths are visualized on a sphere in d_1-d_2-d_3 space (lower left). Only the magnitudes of the flow strength vectors are visualized on the sphere. Once a point on the d_1-d_2-d_3 space is selected (shown as a gray glyph), a test specimen extraction direction from a reference material can be obtained for tri-axial loading test as visualized on the lower right corner.

7 Summary

Because of the complexity of the underlying deformation mechanisms, structural material design is a process dominated by empiricism and trial and error iteration. The complicated relationships between material structure and resultant mechanical properties conspire against the creation of optimization-based material design methodologies. The current state of computational capabilities coupled with the existing materials science knowledge base creates hope for the future of material design, however. Coupled with a new generation of experimental probes that focus on quantification of the mechanical response on multiple size scales, it may soon be possible to understand the optimal material configuration for a specified loading condition. The first step towards realizing this possibility is the creation of a design environment where simulated and experimental data can be employed interchangeably to probe material configuration space. The Digital Material developed in this project is such an environment. The material representation is based on observable features of the internal geometry so that models of different forms and based on different size scales can be employed. Virtual analogues to physical samples can be extracted, loaded and probed in a manner that mimics physical experiments. Properties extracted from the virtual experiments are then stored in an appendix to the database; it is here that the designer can browse various modeling estimations of critical material properties derived from a particular state.

While the Digital Material is largely a software-based material design methodology created to shorten development times by elimination of some physical tests, high fidelity experiments designed to validate and calibrate the multiscale simulations lie at its core.

Acknowledgements/Disclaimer

The authors wish to express their gratitude to several individuals that have contributed to the results of this project. Namely, Chris Pelkie, Cornell Theory Center, for visualization; Linda Buttel and Mike Padula, Cornell Theory Center, for data base design; Alexander Kazimirov, CHESS, and Jim Richardson, IPNS, for their invaluable assistance with the diffraction experiments; and Jun-Sang Park for his work in obtaining EBSD data. This work was sponsored (in part) by the Air Force Office of Scientific Research, USAF, under grant/contract number F49620-02-1-0047. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the Air Force Office of Scientific Research or the U.S. Government.